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RECENT ADVANCES IN CFD-DEM SIMULATION OF FLUIDIZED BEDS

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ABSTRACT

For many decades, experimental measurements, usually at the lab scale, have been considered the main basis for developing and designing commercial-scale gas-solid equipment. However, it is difficult to describe the hydrodynamic characteristics of this flow, despite the extensive experimental work carried out by many researchers. Due to the increasing development of computational performance, numerical simulations are gaining particular importance in the prediction of gas-solid flows, studying design modifications, and complementing experimental data. Although real-time simulations will require substantial progress in the accuracy, capability, and efficiency of numerical models, future developments could herald a new era of so-called virtual reality for process engineering, featuring interactive simulations instead of stepwise experimental scale-up studies and cost-intensive empirical trial-and-error methods. This review provides a significant body of knowledge on the developments of CFD-DEM models and how they can be applied in various gas-solid systems, mainly fluidized beds. Current research trends, as well as research gaps and opportunities for future CFD-DEM applications to chemical and energy processes based on fluidized bed systems, are presented.

Keywords: Gas-Solid Flows; Fluidized Bed; CFD-DEM Model

1. INTRODUCTION

Chemical and energy systems are complex processes that include several phenomena such as thermochemical reactions and multiphase flows. Diverse materials lead to different two-phase flows. In practice, there are gas-fluid, fluid-solid, and gas-solid flows. In gas-fluid flows, one of the phases is in a dispersible form, while in the fluid-solid and gas-solid flows the solid always remains in the dispersed phase.

Experimental measurements enable a fundamental understanding of the hydrodynamic behavior of reactive gas-solid flows, but detailed experimental data is hard to get hold of due to the harsh environment (high temperature, high pressure, and/or toxic gases), and the costs of measuring devices.

Numerical simulation makes it possible to bypass a long process of planning and constructing experiments, providing a quick evaluation of local and global flow field variables (e.g. the temperature, velocity, and concentration) at the industrial scale. However, the reliable simulation of large-scale systems is hindered by a failure to accurately understand the fundamentals of gas-solid flows (e.g. gas-particle, particle-particle, and particle-wall interactions) [1].

Taking into account how the gas phase influences the solid phase and vice versa, as well as how particles influence other particles and walls (gas-particle, particle-particle, and particle-wall interactions), one can differentiate between various coupling approaches, mainly two-way coupling and four-way coupling. There is also a three-way coupling scheme, in which the gas and particle affect each other and the particle wakes and other gas-phase disturbances affect the motion of other particles, e.g. drafting of a trailing particle.

For the representation of gas-solid flows, there are different computational fluid dynamic (CFD) models available, namely the two-fluid model, the discrete-particle model, the hybrid model, and the direct numerical simulation model [2].

2. THEORY

In the discrete-particle method, the gas phase is modeled as a continuum and the solid phase is treated as a dispersed phase, in which individual particles are tracked transiently in the computational domain. The discrete-particle method is distinguished by its particle collision detection methodology, either stochastic or deterministic. The detection of particle-particle and particle-wall collisions is crucially important in terms of both the computational effort and the simulation accuracy.

The idea behind the stochastic collision models is that the motion of each particle is calculated independently of the remaining particles. However, information on other particles should be available to generate virtual collision partners, whose properties are derived from the local average values of these particles. The probability of a collision occurring between the investigated particle and the virtual particle can then be calculated using random numbers. In the deterministic collision detection models, each particle is tested for a possible collision with other partners (particle or wall) [3].

For the discrete-particle simulations with stochastic or deterministic collision detections, two models are widely used for particle-particle and particle-wall collisions, namely hard-sphere and soft-sphere models. The hard-sphere model allows instantaneous and single binary collisions between the collision partners, which are considered to be rigid spheres (or ideal spheres) so that there is no deformation of the particles during the collision. Properties of the particles after the collision (e.g., velocity, position, and temperature) are related to the properties of the particles before the collision through momentum and energy balances.

In the so-called soft-sphere model, also known as the discrete element method (DEM), the particles can overlap each other or penetrate the wall (see Figure 1.) Depending on the penetration depth, a contact force is determined, changing the motions of particles. In this model, a particle-particle collision takes place when the distance between the center points of two particles is smaller than the sum of both radii. Likewise, a particle-wall collision occurs if the distance between the particle center point and the wall surface is smaller than the particle radius. Depending on the penetration depth, the resulting contact force is modeled using a spring-damper-slider system. The most important advantage of the DEM model is that multiple particle-particle and particle-wall collisions can be calculated simultaneously. In addition to contact forces, other short-range forces such as adhesive forces can be taken into consideration in the context of the DEM model.

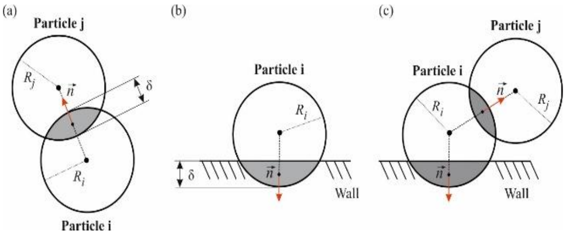

Figure 1. Collision occurrence in the DEM model [4]

In the following sections, we will review the existing literature on the soft-sphere model within the framework of the discrete-particle model, applied to chemical and energy processes based on fluidized bed systems. The CFD-DEM studies found in the literature (with and without chemical reaction) have been evaluated, with a special focus on works that include validation, comparison with other numerical approaches, and their application to real systems.

3. DEVELOPMENT STATUS

Although the DEM model was originally developed by Cundall and Strack [5], in 1993 Tsuji et al. [6] presented one of the first successful DEM simulation studies on the hydrodynamic behavior of gas-solid flows in a lab-scale fluidized bed system. They calculated the trajectory of each particle, taking into account the influence of the gas phase on the solid phase and vice versa, in addition to the particle-particle and particle-wall collisions. This approach is also known in the literature as the DDPM-DEM or CFD-DEM model.

In recent years, significant advances have been achieved in this field of research. Many authors have also compared the simulation results of the DEM model with measurements and with the results of the two-fluid model and the hybrid model, among others, in the works of Chiesa et al. [7]. The DEM model shows better agreement with experimental data compared to other numerical approaches. However, the DEM simulation is computationally expensive when tracking particles in gas-solid flows due to the high computational effort required to detect particle-particle and particle-wall collisions.

A review of the literature on the DEM model reveals that a significant number of published papers are related to cold gas-solid flows, focusing at the early stage of development on 2D and quasi-2D simulations and recently on 3D simulations at the lab scale. Although many authors mention industrial applications in their works, non-reactive gas-solid flows with spherical particles are assumed in most DEM simulations. This simplification is usually accompanied by neglecting a certain number of volume and surface forces, as well as the forces that act on the particles (e.g. Basset, Saffman, Magnus, and electrostatic forces)[8–10].

The drag force makes up a considerable part of all works on DEM and remains one of the major challenges faced in simulations of gas-solid flows. Numerous DEM studies have been carried out using several conventional drag models, such as those developed by Wen and Yu, Syamlal, O’Brien, and Gidaspow. As these conventional drag models have been proven to overestimate the momentum transfer between the gas and solid phases [4], several modifications have been made.

For example, a three-zone or a four-zone drag model calculates the interphase momentum transfer coefficient by selecting universal drag laws for each zone to match the experimental data [11]. Advanced drag models based on flow structures have also been developed, such as the energy minimization multi-scale (EMMS) model or the drag model as described by Kuipers, showing more accurate results regarding the modeling of circulating fluidized bed systems [12–14].

The contact forces are of particular relevance in fluidization systems and are therefore taken into account in all DEM simulations. The contact force is determined using the Voigt-Kelvin model, which describes the viscoelastic and time-dependent behavior of collision[15]. Part of the kinetic energy is irreversibly dissipated in the form of deformation energy and can be taken into consideration by employing restitution coefficients. At higher collision velocities or for a particle with non-spherical shapes, the restitution coefficients decrease and thus cannot be considered constant [16].

However, the restitution coefficients are set as constant in previous DEM studies due to the relatively low particle velocities and the assumption of spherical particles. Although the non-linear contact models show an accurate distribution of the contact force curve, the linear contact model, which consists of a linear spring model and a linear visco-elastic damping element, has frequently been applied [17].

In the literature on DEM, the effect of the adhesive forces without physical contact (e.g., van der Waals and electrostatic forces) is rarely investigated [18]. This is since these forces are of relevance for micro-size particles. Accordingly, the number of fine particles per volume unit is enormous, which in turn makes the DEM simulation of fluidized bed systems with finer particles extremely expensive.

Furthermore, the electrostatic effect significantly decreases at higher temperatures, and parameters such as particle sizes are not used in most fluidized bed applications. At a high moisture level, the adhesive force due to liquid bridging can have a particularly significant influence on the hydrodynamic behavior of gas-solid flows in fluidized bed systems. The simulation of this adhesive force with and without the liquid transport process due to liquid bridge separation has been widely discussed in the literature on DEM[19,20].

Notwithstanding the great efforts and progress made in recent years in the discrete-particle model with DEM, basic flow properties (e.g. segregation, agglomeration, and attrition) are still not taken into consideration sufficiently. Furthermore, real particulate systems include particles of different chemical compositions, densities, shapes, and sizes (e.g. wood pellets or wood chips) that may change during the transient simulation due to chemical reactions.

Most DEM studies in the literature are restricted to circular particles in 2D cases, or spherical particles in 3D cases, which are of constant diameter (monodisperse) and have the same material properties [9]. The fluidization behavior of particles with complex geometries and different material properties is significantly more complicated than that of spherical particles. Furthermore, the heat and mass transfer rates largely depend on particle geometry. Relatively big particles imply larger temperature gradients and have longer residence times. Despite this, limited numbers of CFD-DEM studies on fluidized bed systems with non-spherical particles can be found in the literature [21].

4. LITERATURE REVIEW

The challenges for the simulation of chemical and energy process systems are to combine the gas flow and the homogeneous reactions with the motions of particles with complex geometries and heterogeneous reactions, taking into consideration the temperature distribution inside the particles as well as the momentum, heat, and mass transfer rates between the gas and solid phases. However, work has only just begun on the chemical reaction mechanism in the discrete-particle model with DEM.

Most works found in the literature are dedicated to heat transfer between the gas and solid phases. Few studies are also found on the gasification or combustion process of solid fuels (including biomass or coal), while CO_2 capture technologies and metallurgical or mining processes are much less frequent.

Since 2006, Scherer et al. have been working on the simulation of biomass and waste combustion in a grate firing system by hooking an in-house DEM code with a chemical reaction mechanism in the commercial CFD code “ANSYS-FLUENT” [22,23]. The numerical results show satisfactory agreement with measurements, even though the model has faced a few challenges, making assumptions such as spherical particles and constant temperature distribution inside the particles.

In 2009, Oevermann et al. [24] presented one of the first DEM studies on the wood gasification process in a 2D fluidized bed system. This study was followed in 2013 by the work of Alobaid [25], who developed an in-house CFD/DEM code, known as “DEMEST”, for the numerical simulation of biomass conversion in fluidized beds. Here, gas-particle interactions are studied using new procedures, known as the offset method and the two-grid method. This improves the simulation accuracy by up to one order of magnitude and allows the fluid grid resolution to be varied independently of the particle size. Within the last seven years, there has been only a moderate increase in DEM studies on reactive gas-solid flows in fluidized bed systems [26].

4.1 NON-REACTIVE SIMULATION

4.1.1 Two-dimensional Applications

Since the successful works by Tsuji et al. [6], the number of manuscripts dealing with the fluidized bed simulation using the DEM model has increased sharply. According to the authors, the CFD-DEM model they developed can provide detailed dynamic information at different levels, from the processing equipment to the individual particle. Mikami et al. [27] developed a numerical simulation model to study the fluidization behavior of dry and wet cohesive powder in a two-dimensional fluidized bed system with 14,000 spherical particles. The results showed that the fluidization of wet powder forms agglomerates. Furthermore, the fluctuations in the pressure drop and the minimum fluidizing velocity were lower for dry particles than for wet powder.

The work by Link [8] was extended by Sutkar et al. [28] to investigate the hydrodynamics of gas-solid spouted, fluidized beds with draught plates and liquid injection. The result indicates that for glass particles under dry and wet conditions, the time-averaged particle velocities are similar to quasi-steady-state behavior. Compared to dry systems, lower particle velocities were observed for the wet systems in both the spout and annulus.

Götz [29] developed a parallel DEM simulation code, in which the computational domain is divided into several decompositions and each sub-block is allocated one processor. Based on the model developed by Götz, Alobaid et al. [30] extended the program to include the numerical simulation of gas-solid flow in a fluidized bed. The particle-particle, particle-wall, and gas-particle interactions are modeled by tracking all individual particles. The results showed that the DEM model can accurately predict the hydrodynamic behavior of the gas-solid flow in the fluidized bed. The simulated spatial distribution of solid, the bed height, and the equivalent bubble diameter agree very well with the experiments (see Figure 2).

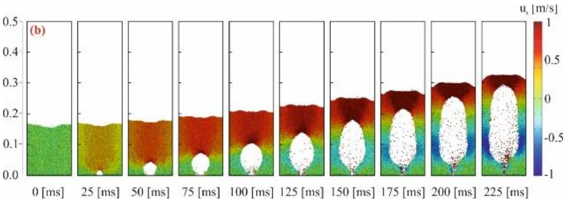

Figure 2. Snapshots of the spatial distribution of solid [30]

Lu et al. [31] investigated how different numerical parameters such as the grid resolution, the drag models (homogeneous and heterogeneous), and the parcel size affected the hydrodynamic behavior of gas-solid flows in a bubbling fluidized bed. The numerical results indicate that the selected drag model has a significant influence on bubble sizes and solid distributions. Progress in recent years was achieved by supplying a pulsed gas mass flow rate to the fluidized bed, the so-called pulsed-fluidized bed (PFB). Wu et al. [32] investigated the dynamic bubble patterns in a quasi-2D pulsed-fluidized bed using the CFD-DEM model. The developed model was validated through experiments, showing quantitative agreement.

Finally, it is worth mentioning that the pseudo-2D CFD-DEM simulations represent a crucial approach for converting the velocity data obtained from particle image velocimetry measurements to the solid flux that provides the most important information for the solid motion in gas-solid fluidized beds.

4.1.2 Three-dimensional Applications

According to the literature, the differences in the solid motions in the 2D and 3D beds are prominent at the beginning of the fluidization process. During fluidization, flow patterns such as the period of bubble formation agree in both simulations, except for the motion of particles near the corners of the bed.

Saidi et al. [33] analyzed the hydrodynamic behavior of gas-solid flows in rectangular spouted, fluidized bed systems of different thicknesses (ranging from pseudo-2D to 3D) using the CFD-DEM model. The results showed that the gas flow fields calculated in the 3D cases have a narrower peak with a higher magnitude of central particle flux compared to the pseudo-2D cases, consistent with measurements. According to the authors, the walls have a considerable impact on the hydrodynamic behavior of gas-solid flows, and this effect becomes insignificant once the thickness increases.

Nikolopoulos et al. [34] compared the coarse-grained discrete-element CFD-DEM with the two-fluid model when both are applied to simulate a semi-industrial riser. The authors explained that the EMMS model and its respective theory were developed and validated based on two-fluid simulations, and it was directly applied to the coarse-grained CFD-DEM model without any modification. The higher accuracy of the EMMS drag model compared with the Gidaspow model was also confirmed.

In most of the studies mentioned above, one component was generally selected for the CFD-DEM simulations, e.g. a riser or a cyclone. The investigated parallelization strategy shows excellent accuracy, good stability, and high efficiency using different processors and under different operating conditions. However, the speed-up ratio and efficiency slightly decrease when the numbers of computational grids and particles are increased.

In this context, Norouzi et al. [35] presented a new parallel CFD-DEM solver that uses both CPU and GPU resources. Using a desktop computer with a 4-core CPU, a frequency of 3.6 GHz, and an NVIDIA GeForce® 660Ti GPU, two different simulation cases were carried out. According to the authors, it took about 6 hours (with two CPU cores) to complete one second of simulation in the case of a large system with 870,000 particles. For the smaller system with 47,000 particles, only 30 minutes (with one CPU core) were required for one second of simulation.

Yang et al. [36] applied the CFD-DEM model for the three-dimensional simulation of a full-loop CFB with six parallel cyclones (see Figure 3). The authors stated that there is a need for full-loop simulations in future works, rather than focusing on a specific component (i.e. the riser) due to the heterogeneous solid loading in the cyclones.

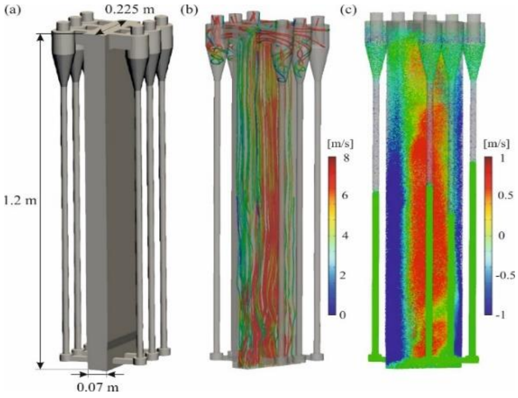

Figure 3. Fluidization behaviour of the gas-solid flow in the full-loop CFB with six parallel cyclones [36]

4.2 REACTIVE SIMULATION

4.2.1 Heat and Mass Transfer Models

In the literature on DEM, there has been broad discussion on specific thermal processes such as the modeling of heat and mass transfer or the consideration of high-temperature adhesive force (metallic solid bridging) in fluidized bed systems. At a sufficiently elevated temperature (60 % of absolute melting temperature), stable solid bridges can be formed between collided particles [37]. The building of sintered bridges depends strongly on the surrounding pressure and the interfacial energies.

Only a few other descriptions were found in the DEM literature, contributing to the agglomeration process. The modeling of heat and mass transfer, by contrast, was discussed in detail. A comparison between the numerical model and the experimental data shows that CFD-DEM simulations are capable of accurately predicting the hydrodynamic behavior of gas-solid flows at elevated temperatures. One example of CFD-DEM simulations with the heat transfer mechanism was presented by Kuipers [38] (see Figure 4).

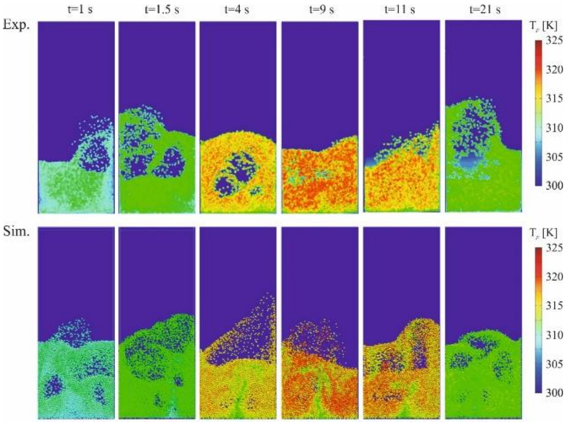

Figure 4. CFD/DEM simulation of a pseudo-2D fluidized bed taking into consideration the heat transfer mechanism [38]

The DEM model that was previously developed to study the heat transfer of spherical particles was extended to evaluate the heat transfer of non-spherical particles. For example, Gan et al. [39] studied the heat transfer in the gas fluidization of ellipsoids. Three heat transfer models (convection, conduction, and radiation) were modified to consider the particle shape and the contact geometry.

The authors claimed that the convective heat transfer coefficients of prolate particles are greater than those of spheres and oblate particles. Wang et al. [40] coupled the CFD-DEM model with a heat exchange model for a single particle, firstly validated for a pseudo-2D bubbling fluidized bed, and secondly applied to a circulating fluidized bed. The numerical results agree with the experimental data in a bubbling fluidized bed. The authors also reported that the gas velocity and particle diameter have a more noteworthy influence on convective heat transfer than on conductive heat transfer.

4.2.2 Combustion and Gasification

Despite the considerable progress in recent years, the CFD-DEM simulation of reactive gas-solid flows in fluidized beds remains a major challenge and is still at an early stage of development. One of the first contributions to this field of research was presented by Zhou et al. [41] in 2004. Here, the DEM model with a large eddy simulation was used to model coal combustion in a 2D bubbling fluidized bed system. The chemical reaction mechanism comprises the heterogeneous reactions of char with O_2, CO, CO_2, NO, and N_2O, along with the homogeneous reactions including CO, O_2, NO, and N_2O. The heat transfer model used took into account particle-gas convective heat transfer, particle-bed radiation heat transfer, the heating rate of a particle, and particle-particle heat transfer.

To reduce the computational cost, Bruchmüller et al. [42] carried out a parallel CFD-DEM simulation on a high-end multiprocessor computer. According to the authors, the superficial fluidization velocity is crucial, while the biomass moisture content is less important for the final bio-oil yield. Alobaid [25] developed a 3D in-house program, “DEMEST”, for the numerical simulation of biomass combustion in a bubbling fluidized bed system (including drying, pyrolysis, and combustion of the char and volatile matter). The numerical results achieve coupling between the CFD-DEM model and the thermochemical reaction mechanism model. The author mentions that the use of other solid fuels such as coal or a mixture of coal and biomass can also be handled with the program.

In another study, Zhao et al. [43] investigated glucose gasification in a supercritical water fluidized bed reactor using the CFD-DEM model. The authors applied a simplified reaction kinetic model, including glucose decomposition, the water-gas shift reaction, and methanation reactions. The numerical results showed good agreement with measurements. It was found that the high wall temperature, the low flow mass rate, and the high initial bed height support the gasification process. At a mass flow rate below the minimum fluidization, the gasification efficiency and thus the H_2 yield decreases.

Directly-irradiated fluidized bed reactors are a promising technology for solar applications (e.g. thermochemical energy storage, solar gasification of hydrocarbons (e.g. coal, biomass, and RDF), and production of solar fuels). Several experimental studies investigated this technology and recently numerical CFD-DEM studies were also performed.

4.2.3 CO_2 Capture Technologies

Various carbon capture processes based on fluidized bed technology are currently being developed (e.g. carbonate-looping process and chemical-looping combustion), but most of them have the consequence of relatively high energy consumption. In the literature on DEM, few studies have been conducted to simulate the chemical-looping combustion process.

The major focus of these works was on investigating the hydrodynamic behavior of cold gas-solid flows in lab-scale systems, while the chemical reaction model was not taken into consideration, e.g.[44,45]. The same applies to CFD-DEM studies used for the carbonate-looping process, with very few exceptions, such as the work of Stroh et al. [46]. According to the authors, the challenges for research lie in the complex hydrodynamics in fluidized beds and the accurate prediction of reactive gas-solid mixtures. They studied the carbonator of the 1 MW_{th} carbonate-looping test facility erected at the Technical University of Darmstadt. The carbonate-looping process, also known as calcium looping, has the potential to significantly reduce the efficiency loss of a conventional steam cycle since the process operates at high temperatures, allowing heat to be used for energy production in a steam cycle. The process can be retrofitted in existing fossil or biomass-fired power plants to remove CO_2 from the flue gas. Furthermore, the technology is particularly suitable for efficiently capturing CO_2 from other industrial sources such as cement or steel plants. Furthermore, different homogeneous drag models (Tang, Gidaspow, Wen and Yu, Syamlal and O’Brien and Gibilaro) and a heterogeneous drag model (EMMS) were applied and evaluated. The authors recommended using the heterogeneous EMMS drag model to improve the accuracy of the simulation result.

For the time being, only a limited number of experimental research works for large or semi-industrial test facilities are available. This is due to the operational challenges in terms of their complexity and the costly measurement apparatus required to obtain the flow characteristics. Therefore, the validated coarse-grained CFD-DEM model at the megawatt scale is of high relevance to upscale the carbonate-looping process.

5. CONCLUSION

A fluidized bed is a bulk of solid particles, with gas flowing into the reactor from the bottom via a porous plate or nozzles. Experimental measurement is usually carried out at a lab scale and provides basic knowledge of the investigated process to underpin design and development. However, the lower costs, the adaptability and the possibility to obtain detailed information are the main reasons why CFD is applied to fluidized bed systems.

Although, CFD-DEM simulations have proven computationally expensive when particles in gas-solid flows due to the high computational cost required to detect particle-particle and particle-wall collisions. A review of the literature on the CFD-DEM model shows that a considerable number of published papers are related to cold gas-solid flows, focusing at the early stage of development on 2D and quasi-2D simulations and recently on 3D simulations at the lab scale. While many authors mention industrial applications in their works, the modeling of turbulence, chemical reaction, and heat transfer is not a part of the CFD-DEM simulation in most cases.

This simplification is usually accompanied by taking into consideration spherical particles and neglecting a certain number of volume and surface forces, as well as the forces that act on the particles. Examples of studies have been reported on fluidization behavior, mixing, and segregation of spherical and non-spherical particles, considering adhesive forces.

It was found that the hydrodynamic behavior of gas-solid flows largely depends on the particles with their complex geometries, size distributions, and material properties. The assumption of monodisperse spherical particles is therefore not valid for the CFD-DEM simulations. However, the CFD-DEM simulations applied to large or semi-industrial test facilities still face major challenges due to the complexity of the process and the computational cost.

All in all, the CFD-DEM model in combination with chemical reactions, heat, and mass transfer may become a standard tool for the design and development of fluidized bed systems. Nevertheless, significant research efforts are required to make the CFD-DEM model as competitive as the present status of the two-fluid model.

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